A Hartree-Fock Study of Persistent Currents in Disordered Rings

A. Kambili*, C. J. Lambert,
School of Physics and Chemistry, Lancaster University Lancaster LA1 4YB, UK

J. H. Jefferson
Defence Evaluation and Research Agency, Electronic and Optical Material Centre, Malvern, Worcs. WR14 3PS UK
(February 1, 2008)

For a system of spinless fermions in a disordered mesoscopic ring, interactions can give rise to an enhancement of the persistent current by orders of magnitude. The increase in the current is associated with a charge reorganization of the ground state. The interaction strength for which this reorganization takes place is sample-dependent and the log-averages over the ensemble are not representative. In this paper we demonstrate that the Hartree-Fock method closely reproduces results obtained by exact diagonalization. For spinless fermions subject to a short-range Coulomb repulsion U we show that due to charge reorganization the derivative of the persistent current is a discontinuous function of U. Having established that the Hartree-Fock method works well in one dimension, we present corresponding results for persistent currents in two coupled chains.
Pacs numbers: 71.30.+h, 05.45.+b, 71.10.Pm, 72.15.Rn

In a normal-metal mesoscopic ring threaded by a magnetic flux [1], measured values of the persistent current [2] are two orders of magnitude larger than predicted. This result suggests that a quantitative theory must treat electron-electron interactions and disorder on an equal footing. Previous studies of spinless fermions concentrated on the behaviour of ensemble averages of the persistent current and led to the conclusion that repulsive interactions cannot significally enhance the current. It was therefore argued that only systems which include spin could show such an increase of the current [3]. However, more recently it was shown [4] that for one-dimensional systems of spinless fermions interacting through a short-range Coulomb repulsion U, the persistent current does increase. This enhancement of the current is accompanied by a charge reorganization of the ground state which happens at different values of the interaction strength U, depending on the disorder realization, and therefore the ensemble averaged persistent current may not be relevant.

The results of [4] were obtained using the density matrix renormalization group (DMRG) technique [5] which is essentially exact and contains correlation effects. However, this technique is computationally demanding and not easily extended to higher dimensions. Therefore it is of interest to determine whether or not the results of [4] are contained in a mean-field description using a single Slater determinant. In this paper we address this question, by presenting results obtained using the Hartree-Fock method for spinless fermions interacting via a short-range Coulomb repulsion. In one dimension we show that the Hartree-Fock method agrees with the exact results of [4], reproducing the predicted behaviour of the persistent current as well as the sample-dependent charge reorganization. After establishing the validity of the method, we extend the calculation to a quasi-one dimensional system comprising two parallel chains.

The total Hamiltonian for a system of N spinless fermions on a disordered chain (1D) of M sites is

$$H = \sum_{i=1}^{M} \varepsilon_i c_i^\dagger c_i - \sum_{i,j=1}^{M} t_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{i,j=1}^{M} U_{ij} c_i^\dagger c_i c_j^\dagger c_j \quad (1)$$

The operators $c_i^\dagger$ and c_i are creation and annihilation operators for an electron on site i, the on-site energies ε_i are random variables uniformly distributed over the interval $-\frac{W}{2}$ to $+\frac{W}{2}$ and U_{ij} is a nearest-neighbour interaction of the form

$$U_{ij} = \begin{cases} U & \text{if } j = i \pm 1 \\ 0 & \text{otherwise} \end{cases} \quad (2)$$

The hopping elements t_{ij} are restricted to nearest neighbours with $t_{i,i\pm1} = t = 1$ except at the ends of the chain, for which $t_{1N} = t_{N1} = 1$ (periodic boundary conditions) or $t_{1N} = t_{N1} = -1$ (anti-periodic boundary conditions).

The single-particle Hartree-Fock equation corresponding to equation (1) is of the form

$$\begin{aligned} \varepsilon_i \Psi^n(i) - t_{ii-1}\Psi^n(i-1) - t_{ii+1}\Psi^n(i+1) \\ + \sum_{m=1}^{N}\sum_{j=1}^{M} |\Psi^m(j)|^2 U_{ij}\Psi^n(i) - \\ \sum_{m=1}^{N}\sum_{j=1}^{M} \Psi^{*m}(j)\Psi^m(i)U_{ij}\Psi^n(j) = E_n\Psi^n(i) \end{aligned} \quad (3)$$

where $\Psi^n(i)$ is the amplitude of the nth single-particle wavefunction on site i. The third and fourth terms are the direct (Hartree) and exhange (Fock) potentials, respectively.

*e-mail: a.kambili@lancaster.ac.uk

The parameters N, M, t, W, and U were chosen to be exactly the same as in [4] so as to directly test the accuracy of the method. Here we present results for $M = 20$ sites and $N = 10$ particles (half-filling) and the strength of the disorder was taken to be large, $W = 9$. At zero U the charge density of a given sample is spatially inhomogeneous due to the presence of such disorder. As U increases we observe a reorganization of the charge, and for large U, obtain a homogeneous configuration in which the particles are equally spaced. This reorganization happens at different values of the interaction strength for different samples. As an example, figure 1 shows the charge density for a single sample in the free electron case ($U = 0$) and for $U = 20$, which is large enough to yield a periodic array of charges.

In addition to the charge density we have studied the phase sensitivity D, which is a measure of the delocalization effect mentioned above and is defined by

$$D(U) = \frac{M}{2}\Delta E \tag{4}$$

Here $\Delta E = (-1)^N(E_g(0) - E_g(\pi))$ is the difference in the ground state energy between periodic and antiperiodic boundary conditions, where the Hartree-Fock ground state energy is

$$E_g = \frac{1}{2}\sum_{n=1}^{N}[E_n + \sum_{i,j=1}^{M} \Psi^{*n}(i)h_{ij}\Psi^n(j)] \tag{5}$$

with $h_{ij} = \varepsilon_i\delta_{ij} + t_{ij}\delta_{ij\pm1}$.

In agreement with [4] we find peaks in $\log D$ at sample-dependent values of U, associated with reorganization of the ground-state charge density. For positive U, figure 2 shows the ensemble average of $\log D$ along with results for four individual samples. For negative U the mean field equations do not converge and no results were obtainable. Fig. 2 is in remarkable agreement with the exact results of [4]. For example the average of $\log D$, exhibits a local maximum around $U \approx t$. Following [4] we have also examined the relative increase of the phase sensitivity with respect to the free fermion case, $\eta = \log D(U) - \log D(0)$, and in agreement with [4], obtain a log-normal distribution for η (figure 3).

Having established the validity of Hartree-Fock theory as a method for computing the charge density and phase sensitivity of one-dimensional rings, we now extend our analysis to two coupled one-dimensional chains. For a system consisting of two rings with 20 sites in each, and 20 spinless fermions in total, we again examine the case of strong disorder, $W = 9$. In figure 4 we show the charge density for the two rings. As we can see, the charge reorganization that was present in 1D is also obvious for two chains. For very strong U the particles localize in the odd and the even sites of the first and second chains respectively, as expected classically. Thus, one again obtains the delocalization effect associated with the crossover from an Anderson to a Mott insulator.

The phase sensitivity and the probability distribution of the relative increase η are shown in figures 5 and 6, which again demonstrate that interactions produce an increase in the fluctuations of the current. However, in contrast with a single chain, the average of $\log D$ no longer possesses a local maximum and instead decreases monotonically with increasing U.

In summary, the above results demonstrate that the effects discussed in [4] are contained in a single Slater-determinant ground state and are describable by mean field Hartree-Fock theory. By extending the analysis to two chains, we find that the maximum in the average of $\log D$ is no longer present, which suggests that this feature may be a peculiarity of strictly one-dimensional systems. The fact that Hartree-Fock theory is applicable in one dimension, where mean field theories are least accurate, indicates that in higher dimensions Hartree-Fock theory should be sufficient to describe the ground state of a system with electron-electron interactions and disorder, at least in the strong disorder limit.

[1] M Buttiker, Y Imry, R Landauer, Phys. Lett. **96A**, 365 (1983)

[2] V Chandrasenkhar, R A Webb, M J Brady, M B Ketchen, W J Gallagher, A Kleinsasser, Phys. Rev. Lett. **67**, 3578 (1991)

[3] T Giamarchi, B Shastry, Phys. Rev. **B 51**, 10915 (1995)

[4] P Schmittekert, R A Jalabert, D Wienmann, J L Pichard, Phys. Rev. Lett. **81**, 2308 (1998)

[5] S R White, Phys. Rev. **B 48**, 10345 (1993)

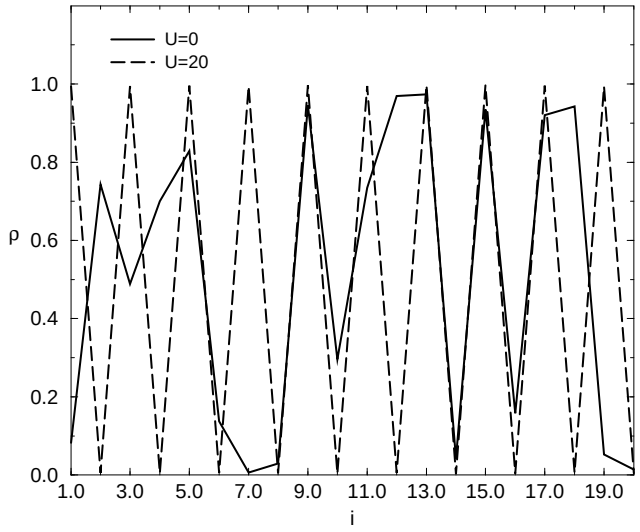

FIG. 1. Charge density for a sample with $N = 10$ particles on a chain (1D) with $M = 20$ sites for free fermions and for $U = 0$ and $U = 20$

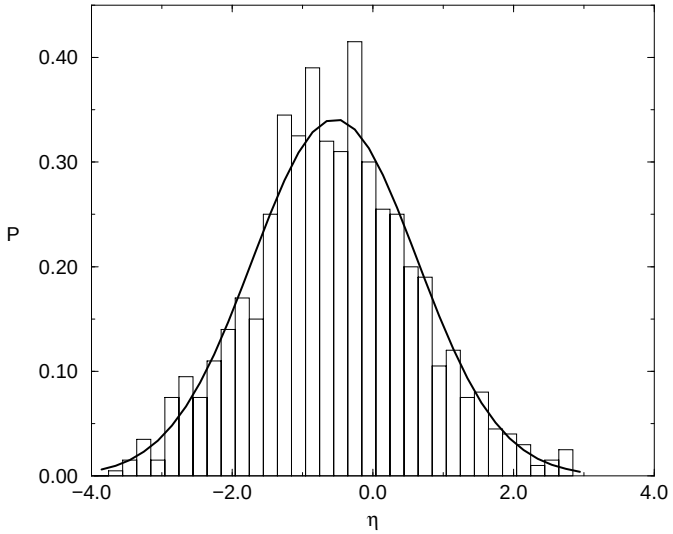

FIG. 3. Probability distribution of $\eta = \log D(2) - \log D(0)$ in 1D calculated from 1000 samples. The curve is fitted by a Gaussian distribution with $< \eta >= -0.53$ and $\sigma^2 = 1.37$

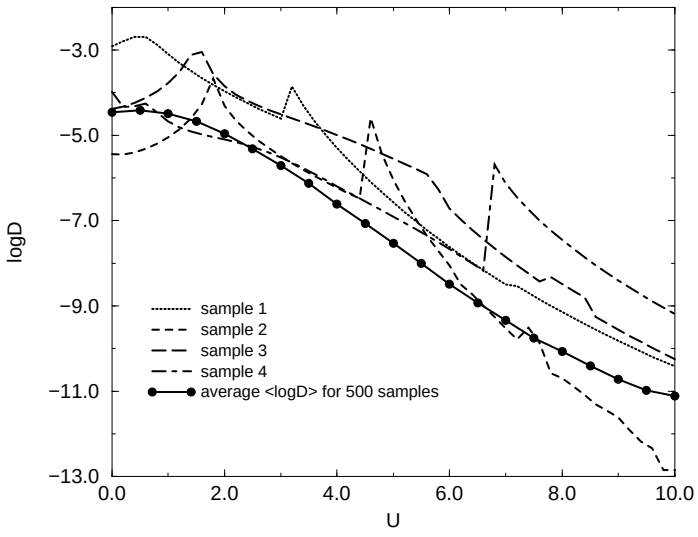

FIG. 2. Phase sensitivity for half-filling ($M = 20$, $N = 10$) in one dimension for four samples. The average has been obtained for 500 disorder realizations

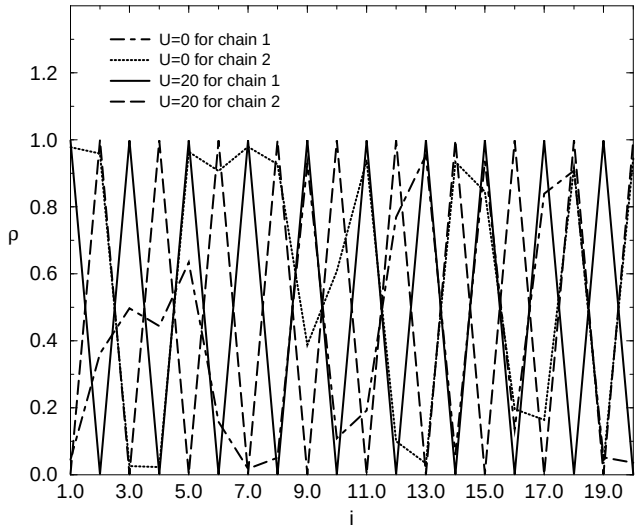

FIG. 4. Charge density for a sample with $N = 20$ particles in two rings (2D) with $M = 20$ sites in each ring for free fermions and for $U = 0$ and $U = 20$

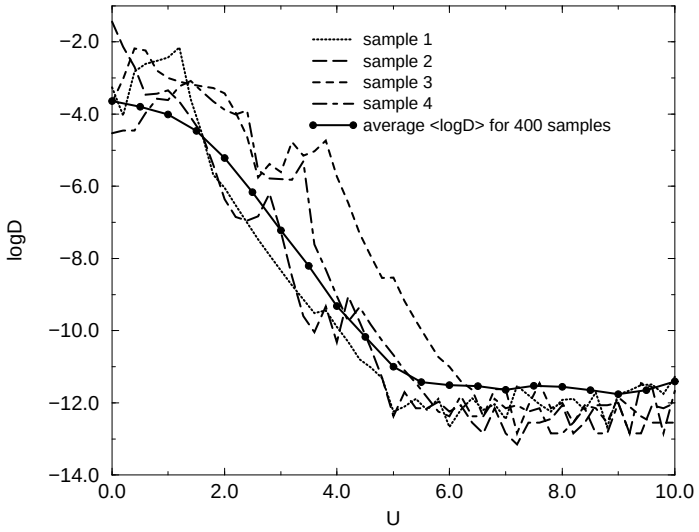

FIG. 5. Phase sensitivity for half-filling ($M = 40$, $N = 20$) in two dimensions for four samples. The average has been obtained from 400 disorder realizations

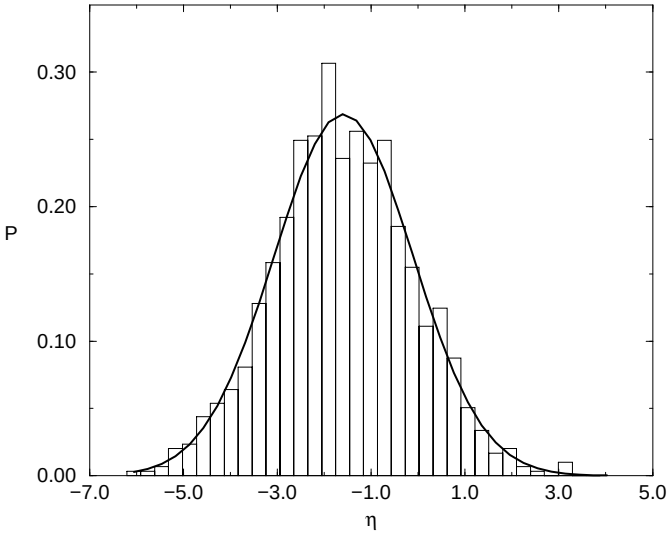

FIG. 6. Probability distribution of $\eta = \log D(2) - \log D(0)$ in 2D calculated from 1000 samples. $< \eta >= -1.59$ and $\sigma^2 = 2.2$